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ANALYTICAL STUDY OF GRAVITY EFFECTS ON LAMINAR DIFFUSION FLAMES

SUMMARY REPORT

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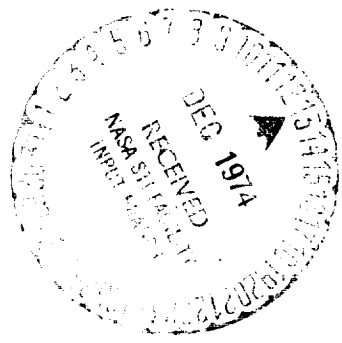

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ABSTRACTS

This report summarizes the progress and problems encountered in the development of analytical tools necessary for the description and aid in interpretation of diffusion flame behavior in low-gravity environments. The report contains a description of the models and the problems encountered. Finally, recommendations for attacking the problems are given.

I. INTRODUCTION

The objective of this study is to develop further understanding of the mechanisms controlling the structure of laminar diffusion flames when affected by gravity. The approach which will be utilized will involve expanding of the analysis developed under NASA Contract NAS3-14378 to include the additional effects of radiation, finite rate kinetics, and axial diffusion under both steady state and transient conditions. The scope of this work shall also include revision of the dimensional analysis developed under the previous contract to reflect the additional effects cited above.

II. AVAILABLE PROGRAM VERSIONS

1. Constant Pressure - (Boundary Layer versions)
   - (a) Chemically Frozen/Finite Rate
   - (b) Complete Combustion
2. Non-Uniform Pressure - (Inclusion of 2nd Momentum Equation)
   - (a) Chemically Frozen/Finite Rate

III. MECHANISMS CONTAINED IN THE MODEL(s)

All versions of the model (1a and b and 2) are described by an axisymmetric, transient formulation based upon approximate forms of the Navier-Stokes Equations, i.e., global continuity, momentum, energy and species equations in their transient compressible form.

Versions 1a and b are based upon a strict boundary layer approximation in which the radial momentum equation is replaced by the assumption that radial pressure variations are zero (as is axial diffusion of mass, energy and momentum).

Version 2 relaxes the assumption on uniform pressure and the radial momentum equation is retained. Each version contains: storage; convection and diffusion of mass, energy and momentum; gravity; finite rate combustion of methane including representations for pyrolysis and soot particle oxidation; and radiation. Variable transport coefficients are also included.

The framework of the model(s) is formed out of the conservation equations and is discussed in References 1, 2 and 3. Reference 1 gives the "boundary layer" type equations in non-conservative form together with the associated finite difference representation using a basic foward time and central space (in x and r) method. The technique is an explicit one.

Reference 2 presents a modification of these equations in the sense of recasting the system into a conservative form and introducing upwind differencing for the finite difference representation of the convective terms. The basic reason for introducing these modifications was to help control conservation and to artifically damp what appears to be excessively large property variations. A problem which seems to be dominant are the large gradients in the near nozzle region which result in extremely rapid timewise readjustments of the "input" initial conditions. Finally, Reference 3 presents an alternate approach based upon the inclusion of the second momentum equation to account for non-uniform pressure effects. In addition to increasing the generality of the model this formulation eliminates the need for density lagging in the conservation equations, (see Reference 1 and 3).

Now, a brief summary of the auxilliary mechanisms included in the model is in order.

Kinetics: The chemical system is assumed to be comprised of the species: O_2,H_2,H_2O,CO,CO_2,CH_4,N_2, A(Argon),H_e(helium) and $C_{(s)}$ (particulate soot). Argon and helium are included to facilitate comparison of the basic kinetics model with available experimental data wherein these species are used as diluents. The kinetics model itself is based upon global rate data from laboratory reactors and is made up of two gas phase oxidation steps, a pyrolysis step, a soot oxidation step and an infinitely fast hydrogen oxidation step (for the H_2 formed out of the pyrolysis of methane). The scheme is uni-directional and is referred to as a subglobal mechanism. The details of the model and examples of the application of it to unit problems are best summarized in References 4 and 5. It should be noted that a standard option available in the program versions containing the kinetics model is chemically frozen flow. This option involves bypassing the kinetics calculation and is applicable to non-reacting flows and situations where it is desirable to compare with the limit of very slow reactions.

Radiation: The radiation model considers the principal emitters to be CO_2,H_2O and soot. It is assumed that the radiating medium is a "gray gas" and that scattering is negligible. The formulation is set in terms of the limiting cases of optically "thick" and optically "thin". These, as well as other assumptions, the describing equations, and the representations used for the required emissivities are given best in References 1, 5 and 6. To date this option has not been exercised within the transient model(s).

Complete Combustion: A version of the "boundary layer" program (1b) contains the complete (or better "quasi-complete") combustion model that has been most widely used in the steady flow "Von-Mises" program. The details are presented in Reference 7, but to date the transient program has not been exercised with this option.

IV. CALCULATION DIFFICULTIES

In Reference 8 results of calculations carried out to a time of 10.5 msec were given using version 1a. The configuration is Test #4 as reported upon in NASA TND-6523, and the initial conditions are based upon the steady state, complete combustion model as used within the "boundary layer" equations in Von Mises coordinates, Reference 7.

As discussed in Reference 8, the transient predictions (which include kinetics) appear reasonable in terms of indicating a small stand-off distance and cool inner core with the flame being open at the tip. Since this calculation is being made under normal-g the physical mechanism contributing to the readjustment of the initial condition is the inclusion of kinetics (in contrast with complete combustion). There is however an additional contribution to this readjustment which is of a numerical nature and is itself a combination of the inherently different solution technique and mesh refinement employed. The relative importance of each of these effects remains to be determined.

In any case, the readjustment that does occur, has had an affect on the manner in which the transient calculation is being performed. In particular, it was found necessary to apply a form of relaxation in order to carry out the calculation without encountering catastrophic failure. The behavior leading to this requirement appears to be manifested

in the global continuity equation wherein the lateral component of velocity (v) is computed. The character of the failure in the calculation was the apparent unbounded growth in the magnitude of v leading ultimately to negative temperatures or species wherein the calculation would self-abort. Inspection of the trends in the computation suggested that this behavior could be suppressed by literally turning off $\partial\rho/\partial t$ in the global continuity equation. This appears to be working in the sense that the calculation can be performed and that the predicted flame structure is settling down to some new steady state configuration (see Reference 8). The fact that $\partial\rho/\partial t$ is not included in the global continuity equation is not in itself distasteful since the normal-g steady state flame is being sought prior to seeking the full zero-g transient flame structure. Nevertheless, it is desirable to turn on the density derivative so that confidence in the calculation using the "full" equations is established. This has been tried at various intervals along the calculation route. Each attempt at turning on the full $\partial\rho/\partial t$ has met with failure which appears to be due to the fact that certain regions in the flow are still adjusting at a relatively rapid rate. At this point $\partial\rho/\partial t$ was relaxed by inserting a partial contribution of it into the global continuity equation. A study was initiated allowing the $\partial\rho/\partial t$ term in the differenced form of the continuity to be 20% of the total contribution to the new v. The results obtained indicate that this procedure is working and by not imposing a sudden large change in v the system responds but begins to settle back down again. It appears that this procedure would permit

the eventual inclusion of the full $\partial\rho/\partial t$ contribution. Concurrently, discussions with the cognizant NASA-Lewis personnel led to another approach which is based upon physical arguments concerning the potential importance of radial pressure gradients in certain regions of the flow particularly during the rapid transient readjustment period. To treat this problem requires the inclusion of the "second" momentum equation which provides the additional equation needed to define the added dependent variable, pressure. The pleasing feature of this formulation is that all variables (u,v,ρ,T and α_i) are determined as a consequence of forward marching in time (as opposed to obtaining the new v without iteration by lagging the $\partial\rho/\partial t$ in the continuity equation in the current "boundary layer" formulation). There is, however, a potential hazard to keep in mind in terms of those regions in the flow where indeed $\partial p/\partial r$ is negligible. Under these circumthe v momentum equation is a higher order equation and the question arises as to the sensitivity (or insensitivity) of the remaining variables of the flow to the v and the p so obtained.

Preliminary calculations using the new formulation (Reference 3) indicate that a sensitivity does exist in terms of the influence that the small pressure variations have on the velocity field. In particular, large accelerations and decelerations (resulting in negative streamwise (u) velocities) are encountered in the near region.

In particular, the revised formulation of the conservation equations including the non-uniform pressure field (Reference 3) has been exercised, and the following studies and observations were made:

1. Several time steps were executed starting at time zero (Von Mises steady state initial conditions) with a) the full system, b) unity Lewis and Prandtl numbers, and c) unity Lewis and Prandtl numbers with frozen chemistry. The observations were as follows:

The results of 1a) show a rapid and large adjustment of flow properties such as temperature in the near region. 1b) and 1c) show nearly the same results as those under 1a). The implication is that diffusion and kinetics contribute a second order change compared with the convective contributions and that the magnitudes of the convective derivatives are possibly not well represented in the grid currently employed. This behavior could be further augmented by the lower order accurate one-sided differencing used in representing these terms. (It should be noted that although all of the above results are essentially the same, 1c does show a slight decrease in temperature as expected.) It should be kept in mind that since the chemistry behaves more like non-reacting flow the question still remains open as to the influence of numerical readjustment upon "quenching" the flow.

2. A long run was attempted starting at time zero but inordinately rapid addition of grid points (spreading) occurred. This was accompanied by a catastrophic distortion of the flow field and the calculation was aborted. A review of the calculation showed that in this case the sympton appeared in the vicinity of the outer boundary involving gross changes in the velocity field. At first it was felt that the rapid adjustments, which are generally observed, had the strongest influence on the regions of lowest velocity (outer boundary). To pinpoint the reason for this behavior we removed the test

on u for adding grid points. We tried this in a short run and it eliminated this outer boundary problem. However, concurrent with this calculation a closer examination of the original run divulged the fact that when grid points were added, the actual pressure p was brought in rather than the "induced" pressure, p'. This was fixed and the need for removing the test on u at the edge was found to be unnecessary.

3. At this point the long run was again attempted. However, the flow field still exhibited relatively large time rates of change with increasingly growing u and v velocities including the occurrence of negative u's. This behavior initiates in the near region and, in accordance with the above, appears to be closely associated with a combination of truncation errors and perhaps local incompatibility between the Von Mises solution and the numerical representation of the transient equations.

On the basis of Item 1 above it appears that the rapid variations in properties (specifically the α_i's and h) arise out of the magnitudes of the convective terms. It is of interest to note that density changes, at least initially in time, are significantly smaller than the corresponding changes in the α_i's and h. It is this behavior that gives rise to large p''s and subsequent large changes in velocity. These changes are sufficiently large such that restoring "forces" are masked. As stated in previous reports the isolated effect of having added kinetics (as compared with complete combustion) needs to be determined.

4. To assess the effect of the p' field upon the velocity field (and the other variables), particularly in the near region, the pressure gradient terms were turned off in both

momentum equations in the first three (3) regions (out to $x = 1.cm.$). The results of this calculation, which went out to 1600 time steps before failure (as opposed to about 25 steps in the basic run) shows that the spatial gradients are better represented by the existing grid yet is still too course.

The sum total of these studies seem to substantiate that poor spatial resolutions aggravated by the inclusion of kinetics are the basic causes for the difficulty.

V. OBSERVATIONS AND RECOMMENDATIONS

For reference purposes the currently available programs are listed below:

1a. Boundary Layer - chemically frozen and finite rate combustion of methane

1b. Boundary Layer - complete combustion

2. Non-uniform pressure - chemically frozen/finite rate combustion of methane

Perhaps the single most important observation made in the application of versions 1a and 2 is the extremely rapid time-wise readjustment of the state of flow in the very near nozzle region. This region of intense activity represents roughly $1/100$ of the domain of interest for the problem under investigation. There are apparently two (2) reasons why this occurs:

1. The near region involves rapid spatial variations in the flow properties. Although the mesh is set-up in zones which are most refined in the near region the adequacy of the refinement has not yet been established. The differences between the numerical techniques used in the "Von Mises" plane (for the steady state initial conditions) and the transient model could easily be magnified in this near region.

2. The second potential cause for the readjustment is a mechanistic one. This is associated with the change in the representation of the chemical reaction mechanism from quasi-complete combustion in the "Von Mises" program to a finite rate mechanism used in the transient program.

To isolate these effects and to determine the overall distortion of the flow field under normalcy conditions, it is recommended that version 1b. be exercised on the current flow configuration. Then, depending upon what is concluded regarding numerically dependent readjustments, appropriate mesh refinements should then be made and evaluated. It should be noted that a "quasi"-complete combustion program of version 2 would be made and evaluated here as well.

There are, in addition, a number of features associated with the numerics that should be evaluated:

First of all, during the course of the development of version 1a of the transient computer programs it appeared that procedures were required to help stabilize the calculations. A direct approach to this problem was adopted and the describing equations were recast into a conservative form while simultaneously central differencing of the convective terms was replaced by "upwind" (one-sided) differences. The former was done to help maintain conservation of momentum, energy and species. The latter was done to better represent the flow of information by accounting for the flow direction. A feature of the "upwind" differencing is that it introduces a fictitious viscosity which can help to stabilize numerical instabilities. However, our studies to date have not demonstrated that such modifications are, in fact, helpful or are required. This needs additional study dictated by the fact that the adequacy of the basic physical mesh (x,r) itself has not yet been established. Reference 9 contains some specific comments relevant to the most recent results which aid in arriving at the summary of recommendations.

VI. SUMMARY OF RECOMMENDATIONS

1. Exercise the "quasi-complete" combustion model, i.e., version 1b.

2. Incorporate the "quasi-complete" combustion model in the revised formulation, i.e., version 2, and exercise.

Now, items 1 and 2 are basically the same in terms of the objective - namely, to isolate numerically driven readjustments from the mechanistic readjustments, i.e. kinetics vs complete combustion. Only relatively short runs would be required to make the assessment.

3. Refine the mesh. Items 1 and 2 above will aid in defining the need for mesh refinement.

4. Evaluate features of the numerical technique
   (a) conservative vs non-conservative form
   (b) central vs one-sided (upwind) differencing. Note that currently the computation assumes that the streamwise component of velocity (u) is always in the positive x-direction. However, our experience indicates that with version 2 (including the induced pressure field) that negative u's are encountered. Therefore provision should be made for true upwind differencing of the streamwise components of the convective terms.

5. Evaluate time step effects. Although preliminary studies involving time step variations indicate that decreasing the step size (below the stability estimate) has little effect, a wide variation is recommended in order to provide conclusive evidence.

6. Although explicit techniques are most common, it is recommended that implicit techniques that are unconditionally stable be examined. One feature of this would be the potentially larger time step that the system could handle.

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